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FINAL REPORT

to

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INTERFACIAL CHEMICAL REACTIONS AND TRANSPORT PHENOMENA IN FLOW SYSTEMS

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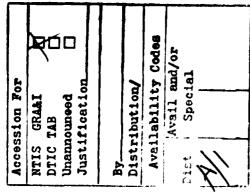
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INTERFACIAL CHEMICAL REACTIONS AND TRANSPORT PRENOMENA IN FLOW SYSTEMS

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Chief, Technical Information Division	





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ABBREVIATIONS								
CT c LBL 1 MIPES m	oundary layer ombustion turbine aminar boundary layer sicrowave-induced clasma emission spectroscopy	QS SCC	Principal Investigator quasi-steady surface catalyzed comb turbulent boundary lay	ustion				

1. INTRODUCTION, OBJECTIVES

<u>Diffusion</u> rates of reactants, reaction intermediates, reaction products and impurites determine the performance of combustion systems — even systems that are premixed and/or turbulent. The existence of large temperature gradients, particularly in laminar (sub-) regions, gives rise to an appreciable thermal diffusion contribution to the "species" mass flux (called <u>Soret</u>-diffusion for vapors, or <u>thermophoresis</u> for particulate matter). This final report reviews, among other things, our recent experimental and theoretical developments on the consequences of thermal diffusion <u>mass</u> transfer in combustion systems, with present emphasis on the behavior of hydrogen in surface-catalyzed-combustion (SCC) and condensate particles (e.g., ash, soot) in a local temperature gradient. In terms of molecular weight disparity (between the transported species and prevailing "carrier" gas) these examples represent important limiting cases, with high molecular weight (e.g., fuel-) vapor transport falling in between.

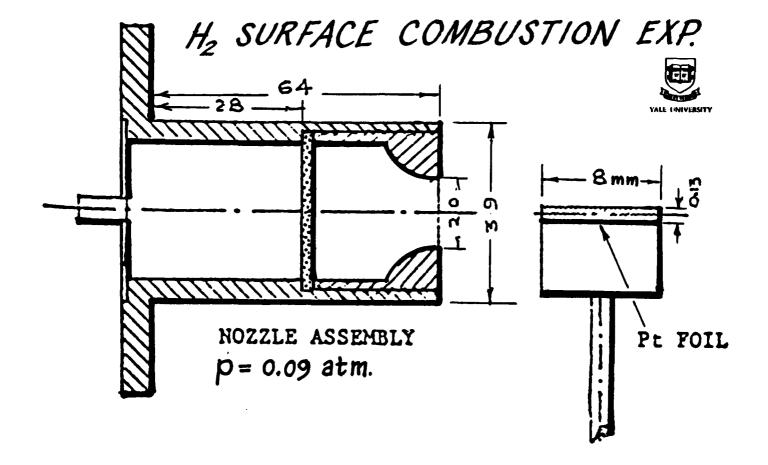
As will be summarized in Sections 2.1 and 2.2, in this research program we have demonstrated several important effects of temperature gradients on diffusional mass transport rates in combustion systems. In general, light vapor species tend to drift toward hot regions/surfaces, and heavy species/particles tend to drift toward cold regions/surfaces. The latter effect is particularly strong, and should also produce some dramatic consequences for small particle nucleation, growth, migration, coagulation and burnout in flames. It is hoped that this research stimulates increased attention to these often neglected phenomena, and their practical consequences in combustion systems. Moreover, our mass transfer research, suitably extended and tested, can be expected to: a) open possibilities for the incorporation of deposition rate criteria in the design/optimization of nextgeneration salt/ash-"tolerant" turbines; b) enable the establishment of sharper minimum performance specifications for all "upstream" fuel treatment, combustion and ash separation systems; and c) suggest rational simulation criteria for laboratory testing of CT blades/materials.

The purpose of this final report is to briefly summarize our research methods and accomplishments under AFOSR Contract F 49620-82K-0020 (Technical Monitors: B.T. Wolfson and J.M. Tishkoff) during the two-year period: 12/1/81-11/30/83. Readers interested in greater detail than that contained in Section 2 are advised to consult the published papers cited in Section 2, and listed in Section 3.1. Copies of any of these published papers or preprints listed in Section 3.1 can be obtained by writing the PI: Prof. Daniel E. Rosner at the Department of Chemical Engineering, Yale University, Box 2159 Y.S., New Haven, CT, 06520, U.S.A. Comments on, or examples of, the applicability of our research results will be especially welcome.

2. RESEARCH ACCOMPLISHMENTS

2.1 Surface-Catalyzed Combustion of Hydrogen

Appreciable effects of Soret (thermal diffusion) transport for hydrogen/air combustion have been predicted for premixed laminar flame structure, and reported in the Russian literature (on surface-catalyzed combustion (SCC)). Our recent SCC-investigations 13, carried out using isothermal calorimetric (power-balance) techniques in the subatmospheric Ptribbon reactor shown in Fig. 2.1-1, reveal that the rate of H₂ transport to an



2.1-1 Detail (schematic) of subatmospheric Pt-ribbon flow reactor for calorimetric studies of surface-catalyzed combustion¹³; reactant gas temperature, Tg, near 300K.

active, hot catalytic surface (e.g., Pt, with $T_w/T_g \approx 3-4$) is systematically increased by more than ten percent (Fig. 2.1-2) by the prevailing temperature gradients. Still larger modifications of vapor mass transport can be expected for H-atoms, or in cases where heavy organic fuel vapors are transported 13.

2.2 Transport of Combustion-Generated Particulate Matter

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2.2.1 Seeded Flame Experiments on Submicron Particulate Transport Rates 2,11

Small particle transport through nonisothermal gases can easily be dominated by thermophoresis, as was confirmed in our recent optical experiments on submicron Mg0-particle deposition from (MgS04-seeded) propane/air flames (Fig. 2.2-1). Relative deposition rates, measured on-line via the loss in Pt-target reflectivity, were obtained at various target and gas temperatures (Fig. 2.2-2) and found to agree with the predictions of thermophoretic LBL theory 3 , 4 (cf. solid curve, Fig. 2.2-2). Moreover, for the same seed level, particle deposition rates at $T_{\rm w}/T_{\rm g}\approx 0.7$ were estimated to be over 1000-times larger than the corresponding rate of convective- (Brownian-) diffusion ($T_{\rm w}/T_{\rm g}$ -insensitive (dashed curve), Fig. 2.2-2). These experiments are now being extended to include soot deposition from fuel-rich premixed flat flames. Preliminary evidence (Section 2.2.2) indicates that soot particle transport to targets or thermocouples is described by the abovementioned laws of particle thermophoresis, although the thermophoretic coefficient of such non-spherical particle aggregates remains to be measured and predicted.

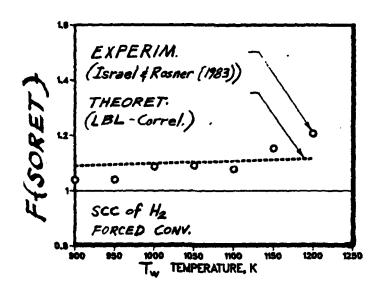
2.2.2 Preliminary Soot Deposition Rate Experiments Using Thermocouple Response Techniques in Rich Hydrocarbon/Air Flat Flames 1

Using transient size and temperature measurements obtained on a small thermocouple bead suddenly immersed in the soot-laden combustion products downstream of a water-cooled flat-flame burner, we have recently demonstrated (via suitable straight line plots (Fig. 2.2-3)) that soot deposition rates are also dominated by particle thermophoresis, i.e., soot particle drift down the temperature gradient prevailing in the gas thermal boundary layer (BL) surrounding the thermocouple target. Observed soot deposition mass fluxes were estimated to be about 100-times greated than those that would have been expected on the basis of only Brownian (concentration) diffusion at the prevailing Reynolds numbers. We concluded that: a) the dependence of the soot deposition rate on temperature "contrast" is in approximate accord with recently proposed thermophoretic BL theories 3,4; and b) the behavior of submicron soot particles in nonisothermal combustion products is strongly influenced by thermophoresis, with important implications for soot coagulation, burnout and deposition.

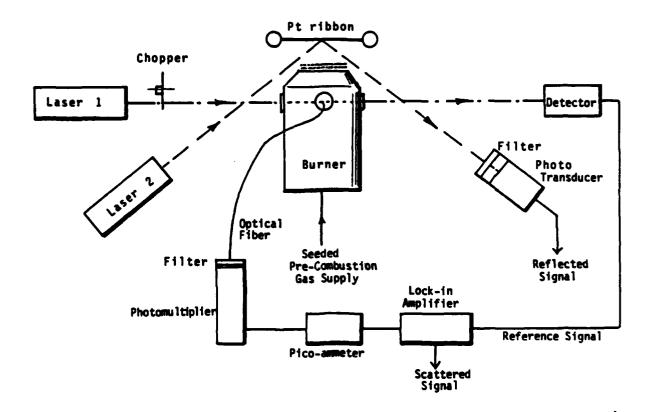
In new soot deposition experiments, initiated during the second year of this program but not yet brought to fruition, we are using laser light scattering techniques to make real-time measurements of soot deposition rates on an actively-cooled stagnation-flow target.

2.2.3 Theoretical Studies of Boundary Layer Transport of Combustion-Generated Particulate Matter

In support of the deposition rate experiments described in Sections 2.1 and 2.2, rigorous boundary layer calculations, including the non-Fickian mass

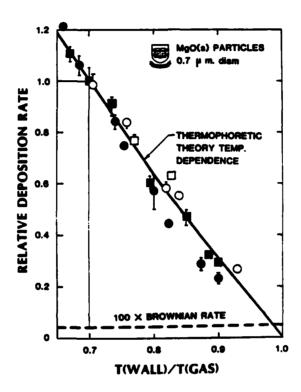


2.1-2: Thermal diffusion (Soret-effect) enhancement of the H₂ transport rate to a Pt-catalyst surface¹³; comparison of experiment with theory^{13,17}.



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2.2-1: Schematic of experimental arrangement for real-time optical reflectivity studies of submicron particle deposition rates from seeded laboratory flat flames^{2,11}.



Comparison of pooled MgO particle deposition rate data (normalized to $T_w/T_g=0.7$) with the T_w/T_g -dependence predicted by thermophoresis-augmented boundary layer theory T(gas)=1500K, T(gas)=1560K, T(gas)=1578K, T(gas)=1585K).

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transfer mechanism of thermal diffusion ("thermophoresis"), have been carried out, and the results used to develop and test simple engineering correlations. As representative outcome of our particle mass transport theoretical studies, Fig. 2.2-4, shows one test of our recently developed correlation4 for rapidly predicting thermophoretically augmented small particle mass transport rates across laminar or turbulent 15,16 nonisothermal boundary layers, including effects of transpiration cooling, and viscous dissipation. Plotted is the ratio of actual mass transfer coefficient (Stanton number) to the corresponding coefficient without particle thermophoresis. Note that, as indeed observed in our experiments (Sections 2.2.1, 2.2.2), temperature gradients can augment the rate of particle capture by over 1000-fold, and our correlation covers a 4-decade range. Over 100 rigorously computed "data" points are shown, with our simple, rational correlation exhibiting an average error of less than 8% in the important parameter range: $0.5 \le T_w/T_g \le 1.0$, $0 \le$ Mach No. <, 10 < Schmidt No. < 106. This research is currently being extended to include: thermophoretically augmented transport of non-spherical aerosol particles (e.g., soot aggregates); implications for both practical combustor deposition and particle sampling from laboratory combustors; effects of advanced surface cooling techniques 7,8 (film and transpiration) on deposition from extreme temperature "dusty" gases; and deposition on surfaces which are hotter than the ambient, particle-laden gas stream.

In closely related theoretical developments, new methods for correlating and extending available <u>inertial</u> impaction information have been developed^{5,6,12}, and can be used to simplify calculations of combustor and turbine fouling in the presence of compressible gas flow, non-Stokes particle drag and inevitable geometric complexity.

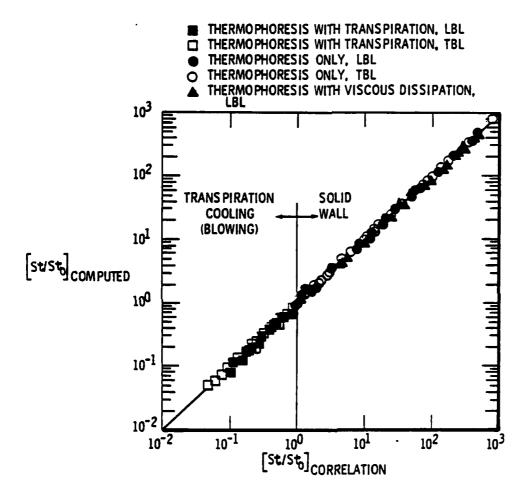
For intermediate size particles the abovementioned diffusional and inertial mechanisms "interact" — indeed, inertial effects can influence diffusional deposition in the absence of actual inertial impaction 14 . A rational conceptual approach to the treatment of such interactions, based on the notion of inertially modified particle concentrations at the mass transfer BL edge, has been developed and illustrated. These results should simplify the problem of accurately predicting the spatial distribution of deposition over a range of intermediate (ca. $l_{\,\,\mu\,m}$ diam.) particle sizes.

Finally, we remark that a portion of our theoretical effort has been devoted to the dynamics of liquid condensate flows on collector surfaces. As a result, aerodynamic shear-driven laminar liquid layers on combustion turbine surfaces can now be predicted. In our current work this theory has been extended to include the simultaneous effects of surface rotation, and the dissolution/corrosion rate consequences of such condensate layer flows on nonisothermal surfaces. It is interesting to note that this work should also apply to thin liquid fuel layers on downstream flame-holders, and at the base of transverse fuel jet injectors.

2.3 <u>Heterogeneous Chemical Kinetics</u>

2.3.1 Chemical and Physical Energy Accommodation at Catalytic Surfaces 10,18

In our previous AFOSR-sponsored research program, to gain a better understanding of the molecular level events which dictate catalyst surface temperatures, we carried out calorimetric measurements on simple heterogeneous



2.2-4: Accuracy of correlations for small particle transport across gaseous boundary layers in the presence of thermophoresis, viscous dissipation and transpiration cooling.

reactions, with emphasis on surface-catalyzed N2H4(g) decomposition. These measurements have now been completed and documented for publication in J. Phys. Chem. 10. A review article outlining the atmospheric chemistry implications of our findings has also been published in Amer. Geophys. Union Monograph No. 2: <u>Heterogeneous Atmospheric Chemistry</u> (1982). Reviewing briefly the contents of Ref. 10, energy transfer to the catalyst per reaction event was studied for hydrazine vapor decomposing on Pt, Ir, or W at T > 900°K. The measurements utilized a newly developed fast-flow chemical reactor which can yield, in a single experiment, values of the chemical energy accommodation coefficient β , thermal accommodation coefficient α for unreacted hydrazine, and the reaction probability Y. Due to the relatively small reaction exoergicity (< 1 ev/molec.) and the great difference between the temperatures of the incident gas and catalyst surface, under the present experimental conditions the reaction becomes endoergic at the catalyst temperature T = 1520 K. We found that above that temperature products depart in thermal equilibrium with the catalyst but below it product molecules carry off 30-40% of the prevailing exoergicity. This result was explained by the desorption of translationally hot H2 product molecules. Incidently, direct desorption of H-atoms contributes to the catalyst energy loss in the case of W above 2000°K.

2.3.2 Development and Application of Microwave-Induced Plasma Emission Spectroscopy (MIPES)

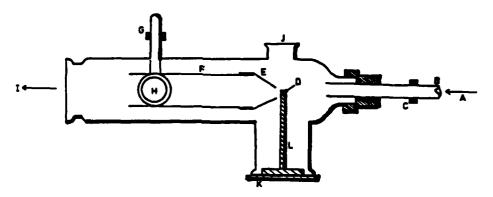
We have recently developed an emission spectroscopic technique which facilitates (i) instantaneous gas/solid reaction rate measurements over a large temperature range in a single experimental run, and (ii) surface mass balances which are necessary for mechanistic understanding of high temperature gas/solid reactions. In this technique, a low-pressure microwave-induced plasma (MIP) excites characteristic emission from the atoms in the gaseous product species of the gas/metal reaction in a low pressure flow reactor. It should be noted, that, while MIP systems have received much attention as spectrochemical excitation sources in the past, this work is evidently the first to make use of the analytical capabilities of MIPs to study the kinetics of high-temperature gas/solid reactions.

We employ a modified version of the transonic, vacuum flow reactors (Fig. 2.3-1) developed earlier under AFOSR-support for the study of gas/solid reactions by Rosner and co-workers 20-22. However, now the reaction product vapor species are dissociated and electronic emission from the resulting atoms is produced in a second microwave discharge plasma (G) before leaving the reactor. Evaporation and gasification reactions are studied by measuring emission intensity from this discharge, <u>via</u> a quartz window, a 75mm-focal-length condensing lens and a 0.5m Jarrell-Ash monochromator.

Aside from steady-state reaction rate measurements, flash evolution experiments can be carried out to measure the amount of condensed product material formed on a surface during reaction provided, of course, that the reaction product has a higher volatility than that of the substrate. In such experiments the filament is exposed to the gaseous reagent for some reaction time (normally only a few minutes). Then, the gaseous reagent flow into the reactor is stopped and the filament cooled to near 300K. Finally, the I(t) is determined when the filament is heated rapidly. The skimmer and the inner coaxial tube shown in Fig. 2.3-1 were installed so that the system detects only products from the central, uniform-temperature region of the filament. Valves

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A, reactant and inert gas mixture;

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B, alumina tube; C, microwave cavity; D, electrically heated specimen filament; E, aluminum skimmer; F, pyrex annular tube; G, microwave cavity; H, quartz observation window; I, to pump, manometer, and throttle valve; J, pyrometer sight tube; K, specimen probe; L, electrical leads and voltage taps to measure specimen resistance.

2.3-1: Transonic flow reactor for kinetic studies of gas/solid (filament) surface reactions using the method of microwave-induced plasma emission spectroscopy (MIPES)¹⁹.

are provided to divert the gaseous reagent to the reactor exhaust or to allow it to pass through the reactor during such "flash evolution" experiments.

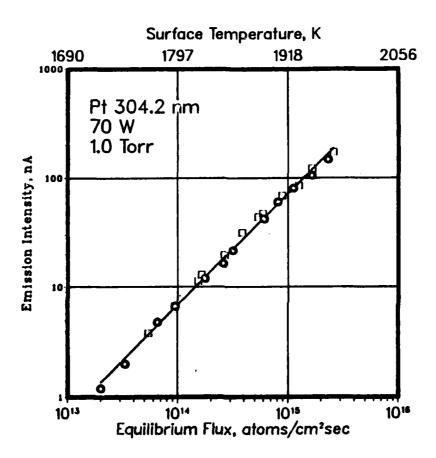
While exploratory flash evolution experiments are now being carried out for the F(g)/Pt(s) system we first demonstrated the capability of MIPES to rapidly and quantitatively follow low metal fluxes by examining the sublimation rate of platinum, using the 304.2 nm line of the Pt(g)-emission spectrum. Figure 2.3-2 reveals that over more than a 2-decade range of metal atom fluxes (starting at only about 2 x 10^{13} atoms/cm²sec) the Pt emission intensity and Pt-flux are directly proportional to one another, as required to exploit MIPES for future gas/solid kinetic studies. Of special interest will be the application of this MIPES-technique to the oxidation of boron, a system of considerable interest to the propulsion community but one whose poorly understood kinetics are apparently influenced by the condensibility of the reaction product $B_2O_3^*$.

3. COMMUNICATION OF RESEARCH RESULTS

3.1 Papers Submitted, Published

- P1. Eisner, A.D. and Rosner, D.E., "Soot Particle Thermophoresis in Non-Isothermal Combustion Gases," 20th Symposium (Int.) on Combustion (submitted, January, 1984).
- P2. Rosner, D.E. and Kim, S.S., "Optical Experiments on Thermophoretically Augmented Sub-Micron Particle Deposition Rates from Dusty High Temperature Gas Flows," Chem. Engrg. J. (in press, 1984).
- P3. Gokoglu, S.A. and Rosner, D.E., "Thermophoretically-Augmented Forced Convection Mass Transfer Rates to Solid Walls Across Non-Isothermal Laminar Boundary Layers," AIAA J. (submitted, 1983).
- P4. Gokoglu, S.A. and Rosner, D.E., Int. J. Heat and Mass Transfer <u>27</u>, 639-645 (1984).
- P5. Rosner, D.E., Gokoglu, S.A. and Israel, R., in <u>Fouling of Heat Exchanger</u> Surfaces, Engineering Foundation, NY (R. Bryers, ed.), 235-256 (1983).
- P6. Rosner, D.E. and Fernandez de la Mora, J., "Discussion of Boundary Layer Effects on Particle Impaction and Capture," ASME Trans.—J. Fluids Engrg. (in press, 1984).
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- P8. Gokoglu, S.A. and Rosner, D.E., "Thermophoretically Enhanced Mass Transport Rates to Solid and Transpiration-Cooled Walls Across Turbulent (Law-of-the-Wall) Boundary Layers," <u>Ind. Engrg. Chem./Fundamentals</u> (in press, 1984).

^{*} This system has some features in common with the 0,N/Si(s) system we studied under AFOSR-support²³ in 1968-1969. That paper²³ proved useful in the design of the NASA Space Shuttle Orbiter Vehicle leading edge system.



2.3-2: Microwave-induced Pt emission line intensity, I, in filament wake vs. equilibrium Pt flux for steady-state Pt(s) sublimation 19.

- P9. Rosner, D.E., Gunes, D. and Nazih-Anous, N., Chem. Engrg. Communications 24, 275-287 (1983).
- P10. Kiela, J.B., Halpern, B.L. and Rosner, D.E., "Chemical and Physical Energy Accommodation in the Metal Surface-Catalyzed Decomposition of Hydrazine Vapor," <u>J. Phys. Chem</u>. (in press, 1984).
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- P16. Rosner, D.E. and Fernandez de la Mora, J., in <u>Particulate Laden Flows in Turbomachinery</u> (W. Tabakoff, C.T. Crowe and D.B. Cale, eds.) ASME, NY, 85-94 (1982).
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- P23. Rosner, D.E. and Allendorf, H.D., J. Phys. Chem. 74, 1829-1839 (1970).

3.2 <u>Verbal Presentations</u>

T1. Rosner, D.E., "Particle and Vapor Mass Transport Through Non-Isothermal Combustion Gases, with Applications to Deposition, Sampling and Surface-Catalyzed Combustion," Eastern States Section-Combustion Inst., Fall '83 Conference, Nov. 8-10, 1983, Brown Univ., Providence, RI.

- T2. Sorge, F., Eisner, A.D. and Rosner, D.E., "Deposition of Nonspherical Soot Particles on Cooled Solid Targets," Final Conference, Yale Engrg. and Applied Sci. Summer Research Program, August 18, 1983, New Haven, CT.
- T3. Rosner, D.E., "Recent Research on the Laws Governing Vapor and Particle Vapor Deposition from Combustion Gases; Implications for Diminishing Deposition in the Direct Firing of (Beneficiated-) Coal in Combustion Turbines," invited panel discussion; presented at EPRI Conference on Combustion Turbine Systems Modification for Direct (Beneficiated-) Coal Firing, August 3, 1983, Palo Alto, CA.
- T4. Rosner, D.E., "Recent Advances in the Field of Vapor and Particle Mass Transfer, with Application to the Fouling of Heat Exchanger Surfaces and Combustion Turbine Blades," Chem. Engrg. Seminar; State Univ. of NY, April 20, 1983, Buffalo, NY.
- T5. Rosner, D.E., "Similitude and Correlation Methods in Transport Processes Some Instructive Non-Equilibrium Examples," Mech. Engrg. Dept. Colloquium, Ben Gurion Univ., Dec. 26, 1982, Negev, Israel.
- T6. Rosner, D.E., "Recent Advances in the Theory of Particle Deposition, with Application to the Fouling of Gas Turbine Blades and Heat Exchanger Surfaces," Aero. Engrg. Dept. Colloquium, Technion-IIT, Dec. 22, 1982, Haifa, Israel.
- T7. Rosner, D.E., "Similitude and Correlation Methods in Transport Processes Some Instructive Non-Equilibrium Examples," Chem. Engrg. Colloquium, Technion-IIT, Dec. 8, 1982, Haifa, Israel.
- T8. Rosner, D.E., "Dynamics of Laminar Condensate Films on Fixed and Rotating Surfaces, with Application to Molten Slag or Salt Films on Combustion Turbine Blades," Fluid Dynamics Research Seminar, Technion-IIT, Dec. 5, 1982, Haifa, Israel.
- T9. Rosner, D.E., "Optical Studies of Dew Points and Deposition Rates from Combustion Gases Containing Inorganic Impurities," Aero. Engrg. Dept.-Combustion Research Seminar, Technion-IIT, Nov. 26, 1982, Haifa, Israel.
- T10. Rosner, D.E., Gokoglu, S.A. and Israel, R., "Rational Engineering Correlations of Diffusional and Inertial Particle Deposition Behavior in Non-Isothermal Forced Convection Environments," presented at the Engrg. Foundation Int. Conf. on the Fouling of Heat Exchanger Surfaces, Oct. 30-Nov. 5, 1982, White Haven, PA.
- T11. Forbes, K.R., Rosner, D.E. and Gunes, D., "Theory of Deposit Formation on Combustion Turbine Blades," Final Conference, Yale Engrg. and Applied Sci. Summer Research Program, August 19, 1982, New Haven, CT.

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T12. Rosner, D.E. and Fernandez de la Mora, J., "Correlation and Prediction of Thermophoretic and Inertial Effects on Particle Deposition Across Non-Isothermal Turbulent Boundary Layers," presented at the ASME-AIAA 1982 Spring Fluids Engrg. Conf., June 7-11, 1982, St. Louis, MO.

4. ADMINISTRATIVE INFORMATION, PERSONNEL

Table 4-1 summarizes the personnel who have contributed to this research program during the period: 12/1/81 - 11/30/83, along with subject matter of each investigator's research contribution. With the exceptions of our summer research assistants (K. Forbes, F. Sorge) and A. Oner, whose work (Section 2.3.2) remains to be prepared for publication, these individuals comprise the PI's co-authors for the papers listed in Section 3.1.

TABLE 4-1

RAMB .	STATUS & YALE U.	PRIMARY CONTRIBUTION
ROSNER, D.E.	PIa, Fac. (ChE)	overall program direction
Anous, N.	GRA ^b (MS program)	condensate layer fluid dynamics
Eisner, A.D.	PDRA	soot-particle deposition rate experiments
Fernandez de la Mora, J.	Fac.(ME)	BL theory of particle transport
Halpern, B.	Fac.(ChE)	chemical and physical energy accommodation
Gokoglu, S.A.	GRA	BL theory of particle transport
Israel, R.	GRA	surface-catalyzed combustion
Kim, S.S.	PDRAC	Mg0-particle deposition rate experiments
Nagarajan, R.	GRA	condensate layer fluid dynamics
Oner, A.	GRA	microwave-induced plasma emis- sion spectroscopy
Sorge, F.	SRPd	soot particle deposition rate experiments

a Principal Investigator

C Postdoctoral Research Assistant

b Graduate Research Assistant

d Summer Research Program
Yale Engineering and Applied Science

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REACTORS, INERTIAL IMPACTION, OPTICAL METHODS, SOOT,									
This report summarizes Yale-High Temperature Chemical Reaction Engineering Laboratory methods/results (contract F49620-82-K-0020) for the two-year period ending 11/30/83. Noteworthy findings on interfacial chemical reactions and mass transport include: 1) thermal (Soret) mass transfer can systematically enhance H2-transport rates to catalytic combustion surfaces by up to 20% in forced convection systems; 2) For submicron particle transport (MgO) to cold surfaces in hot combustion gases thermophoresis causes about a 2000-fold increase in the deposition gate (over that expected from convective-(Brownian) diffusion); 3) By accounting for the "suction" and apparent-source effects associated with thermophoresis within particle laden nonisothermal boundary layers (BLs) simple rational engineering correlations have been proposed and verified via numerical laminar and turbulent BL-boundary calculations; 4) Quantitative, rapid-response measurements of solid gasification kinetics have now been made using an adaptation of microwave-induced-plasma emission spectroscopy. This technique, shown to follow Pt-atom fluxes down to ca. 2 x 10 ¹³ atm/cm ² /s. 20. DISTRIBUTION/AVAILABILITY OF ABSTRACT VINCLASSIFIED UNCLASSIFICATION UNCLASSIFICATION UNCLASSIFIED Unclass									
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18. SUBJECT TERMS (CONTINUED)

THERMAL DIFFUSION, THERMOPHORESIS and TURBINE BLADES.

19. ABSTRACT (CONTINUED)

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